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AI-driven optimisation of drug delivery systems for therapeutic enhanced efficacy

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By guaranteeing that medicinal materials reach the intended spot in the body with maximum efficacy and few side effects, drug delivery systems (DDS) are essential to modern medicine. However, time-consuming and expensive trial-and-error methods are frequently used in traditional drug delivery systems. Predictive modelling, formulation optimisation, and tailored therapy have all been made possible by the development of artificial intelligence (AI), especially machine learning and deep learning, which have drastically changed pharmaceutical research. This study examines how AI-assisted optimisation affects therapeutic results in drug delivery systems. Advanced drug carrier design, pharmacokinetic and pharmacodynamic behaviour prediction, and real-time drug release monitoring are all made possible by AI technologies. Additionally, specialized delivery methods like nanoparticle-based carriers, which increase drug bioavailability and lower toxicity, are made possible by AI-driven models. AI has a lot of promise, but there are still issues with data quality, regulations, and model interpretability. Future medication delivery is anticipated to be revolutionized by the integration of AI with digital health platforms, nanotechnology, and precision medicine. This study highlights important technologies, applications, difficulties, and opportunities while examining the function of AI-assisted optimization in drug delivery systems and assessing its potential to enhance therapeutic outcomes.

Keywords: *Artificial intelligence, drug delivery systems, machine learning, nanomedicine, personalised medicine, therapeutic optimization*

Introduction

For medications to be supplied efficiently, safely, and at the proper dosage, drug delivery systems are crucial. Empirical experimentation, which can be expensive and time-consuming, is a major component of traditional drug development techniques. The demand for more effective and predictive approaches to medication delivery design has grown as current medicines become more sophisticated. A potent instrument that has the potential to revolutionise pharmaceutical research and development is artificial intelligence (AI). Large biological and chemical datasets may be analysed, trends can be found, and drug action within the human body can be predicted thanks to AI technologies like machine learning (ML), deep learning (DL), and data-driven modelling. These features make it possible to create drug delivery systems that are tuned to improve therapeutic results and reduce adverse effects (Ros et al., 2026). The use of AI in drug delivery has been further increased by recent developments in biomedical engineering and nanotechnology. Artificial intelligence algorithms can model drug-biological system interactions, optimizing drug loading efficiency, and predicting nanoparticle features. More specialized and individualized treatments are now possible because to these advancements (Singh & De, 2026).

Overview of drug delivery systems

An overview of drug delivery systems is shown in Figure 1, which highlights the various techniques for efficiently delivering drugs into the body. It emphasises popular methods such as transdermal distribution (patches, gels, and lotions applied to the skin), injectable delivery (including IV injections, microneedles, and implants), and oral delivery (tablets and capsules ingested by mouth). Additionally, the infographic highlights cutting-edge technologies like liposomes and nanoparticles, which function as tiny carriers to enhance drug stability, targeting, and controlled release. Furthermore, it has been demonstrated that targeted drug delivery methods, such monoclonal antibodies and ligand-conjugated medications, can transport medication straight to cells or tissues, minimizing side effects. Additionally covered are cutting-edge developments like hydrogels, nanorobots, gene therapy, and biodegradable implants, which show how contemporary pharmaceutical research is creating more accurate and effective drug delivery methods for better therapeutic results (Patra et al., 2018; Zhu et al., 2025).

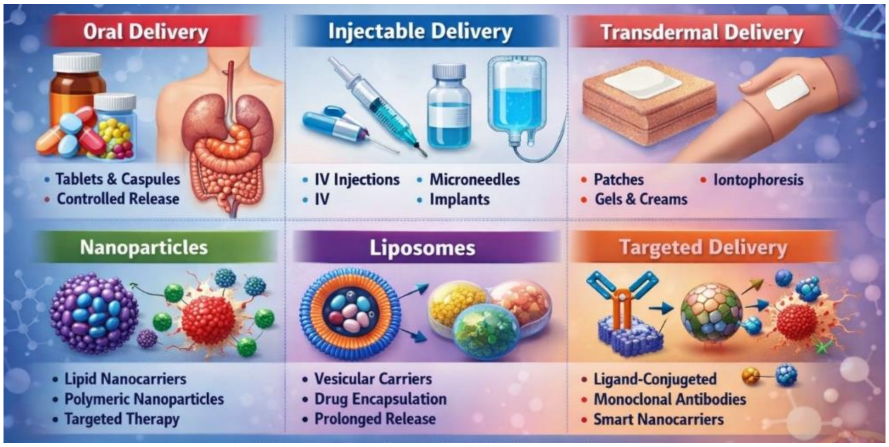

Figure 1. Overview of drug delivery

Drug delivery systems are technologies that deliver therapeutic drugs in a regulated way to the body. Enhancing therapeutic efficacy, reducing side effects, and increasing drug bioavailability are the main goals of DDS. Oral tablets, injections, and topical preparations are examples of conventional medication delivery methods. However, these traditional approaches frequently have drawbacks such systemic toxicity, fast drug breakdown, and limited absorption.

Among the contemporary drug delivery methods are:
• Nanoparticle-based delivery systems
• Liposomes and polymeric carriers
• Controlled-release formulations
• Targeted drug delivery systems

Systems for delivering drugs specifically because they can deliver medications directly to sick tissues while lowering systemic exposure, nanoparticle drug delivery methods have garnered a lot of interest. However, rigorous control over factors including particle size, surface chemistry, and drug loading capacity is necessary to build the best nanoparticle carriers. AI technologies can help optimize these parameters by analysing complex datasets and predicting the best formulation strategies.

Role of artificial intelligence in drug delivery optimization

Table 1. Comparison of AI techniques in drug delivery

AI Technique	Key Features	Applications in Drug Delivery	Advantages	Limitations
Machine Learning (ML)	Learns patterns from experimental data	Drug formulation optimisation, prediction of drug release profiles	Reduces experimental trials	Requires large datasets
Deep Learning (DL)	Neural networks with multiple layers	Molecular structure analysis, nanoparticle design	High prediction accuracy	Computationally expensive
Reinforcement Learning	Learns through reward-based optimization	Adaptive drug dosing systems	Dynamic optimization of treatments	Complex training process

Natural Language Processing (NLP)	Extracts information from scientific texts	Literature mining, drug discovery databases	Speeds up knowledge extraction	Limited by quality of literature data
Predictive Modeling	Uses statistical and computational models	Pharmacokinetic and pharmacodynamic prediction	Improves dosage accuracy	Requires validated models

Researchers can examine massive datasets, spot trends, and forecast the best medicine delivery methods thanks to AI technology's potent computational capabilities. Researchers can greatly enhance patient safety, therapeutic efficacy, and drug formulation design by combining AI algorithms with pharmaceutical sciences. AI methods for analysing complicated biological and pharmacological data include machine learning, deep learning, and predictive modelling. These methods allow scientists to investigate the connections between biological reactions, carrier materials, and medication composition. In the discipline of pharmacology, where comprehending how medications interact with biological systems is crucial for creating successful treatment plans, this kind of analysis is very significant. Table 1 provides a concise comparison of major AI techniques used in drug delivery, highlighting their core functions, strengths, and application areas. It outlines how methods like machine learning, deep learning, and reinforcement learning differ in predictive capability, adaptability, and therapeutic optimisation (Vora et al., 2023).

Machine learning for drug formulation design

By evaluating experimental datasets and identifying optimal combinations of active pharmaceutical ingredients and excipients, machine learning algorithms are frequently used to optimise drug formulations. The effects of formulation parameters on drug stability, solubility, and release kinetics can be predicted by these methods. Machine learning significantly accelerates drug development by eliminating the need for lengthy laboratory trials (Vora et al., 2023). To anticipate the best formulation parameters for novel drug candidates, for instance, supervised learning algorithms can be trained using past pharmaceutical data. These models enable researchers to determine the most effective medication delivery techniques by evaluating several formulation variables at once (Ros et al., 2026).

Predictive modelling of pharmacokinetics and pharmacodynamics

Drugs' passage through the body and interactions with biological targets are described by pharmacokinetics (PK) and pharmacodynamics (PD). Complex PK-PD datasets can be analysed by AI systems to forecast the effects of various drug delivery methods on treatment results. Researchers can model drug absorption, distribution, metabolism, and elimination processes using AI-driven PK-PD modelling. These simulations aid in determining the best dosage schedules and enhance medication effectiveness while lowering side effects. In personalised medicine, where treatment plans must be customised for each patient, these prediction skills are very helpful (Topol, 2019).

Deep learning for molecular and nanocarrier design

Deep learning methods process complex biomedical data using multi-layered artificial neural networks. Deep learning is especially helpful in drug delivery research for creating nanocarrier-based delivery devices and evaluating molecular structures. The interactions of nanoparticles with biological tissues and cellular surroundings can be predicted by computational models. Drug delivery methods based on nanoparticles have grown in significance for focused treatment, particularly for illnesses like cancer. AI models can assist in creating nanoparticles with ideal characteristics, such as drug loading capacity, size, and surface charge. This minimises harm to healthy tissues while enabling accurate targeting of sick cells (Kantesaria & Panda, 2026; Singh & De, 2026).

AI-assisted optimisation of drug delivery systems

Figure 2 illustrates how AI can improve pharmaceutical medication delivery systems to improve therapeutic outcomes. The process begins with data collection and analysis, which entails obtaining biological, clinical, and molecular data from patient records, laboratory studies, and biomedical databases. This data is then processed via AI model building, which includes machine learning, deep learning, and prediction algorithms that look for patterns and links in the data. AI approaches support drug formulation design, pharmacokinetic and pharmacodynamic (PK/PD) modelling, and nanoparticle structural optimisation for efficient drug transport in the following stage: optimisation and simulation.

Finally, the application of the enhanced models to drug delivery applications enables targeted therapy, personalised medicine, and intelligent drug delivery systems (Chou et al., 2025).

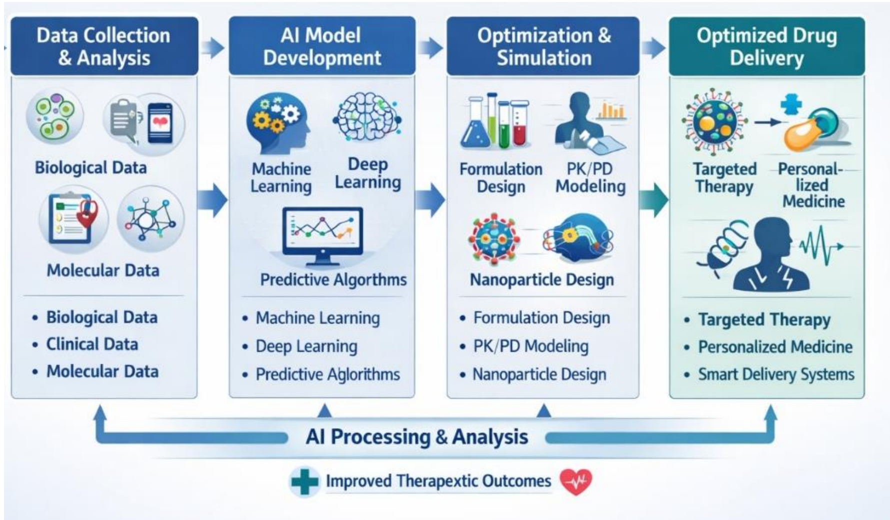

Figure 2. AI-assisted drug delivery systems

Formulation design and optimisation

Artificial intelligence (AI) systems can evaluate trial datasets and find correlations between formulation factors and therapeutic performance to establish the best medication formulation parameters. These models help researchers identify the best excipient, polymer, and active pharmaceutical component combinations. For instance, machine learning algorithms can forecast how formulation modifications affect drug release patterns, stability, and therapeutic efficacy. AI-driven models can greatly reduce the number of experimental trials needed during formulation development and speed up the entire drug discovery process by analysing massive pharmaceutical datasets (Vamathevan et al., 2019).

Pharmacokinetic and pharmacodynamic modelling

Pharmacodynamics (PD) explains how medications interact with biological targets, whereas pharmacokinetics (PK) discusses how drugs travel through the body. AI-based models can forecast how various drug delivery methods affect treatment results and simulate PK–PD correlations. Researchers may more precisely examine medication absorption, distribution, metabolism, and excretion processes thanks to these computational techniques. AI-assisted PK–PD modelling thus aids in improving therapeutic efficacy, minimizing adverse drug reactions, and optimising dosing schedules. Precision medicine uses these predictive modelling approaches more to customise treatments based on the unique characteristics of each patient (Mak & Pichika, 2019; Wang et al., 2025).

Nanoparticle design

Because they may target certain tissues and increase medication bioavailability, nanoparticle-based drug delivery methods have garnered a lot of interest. The behaviour of nanoparticles in biological contexts, such as cellular absorption, biodistribution, and toxicity, can be predicted with the aid of AI technology. To create more effective nanocarriers, machine learning algorithms can examine the physicochemical characteristics of nanoparticles, such as particle size, surface charge, and drug loading capacity. These predictive models expedite the development of sophisticated drug delivery systems, lower experimental costs, and increase the efficiency of nanoparticle design. AI-powered nanoparticle design has demonstrated potential uses in tailored treatments for illnesses, including cancer (Mitchell et al., 2021; Kaur et al., 2025).

Applications of AI optimised drug delivery

AI-Optimised Drug Delivery Applications Artificial intelligence improves contemporary drug delivery methods in several medical applications, as seen in Figure 3. Targeted cancer therapy, personalised medicine, smart drug delivery technologies, and controlled-release formulations are the four main fields shown in the illustration. AI aids in the creation of nanoparticle carriers that deliver medications straight to tumour cells in targeted cancer therapy, increasing the efficacy of treatment for illnesses like cancer while reducing harm to healthy organs. Precision medicine's tenets are supported by personalised medicine, where AI evaluates patient-specific clinical and genetic data to create customised medication compositions and treatment regimens (Mamoshina et al., 2016). To monitor physiological signals and modify medicine dosage in real time, smart drug delivery systems combine biosensors and artificial intelligence algorithms. This is especially helpful for managing long-term illnesses like diabetes. Additionally, by improving polymeric drug carriers to guarantee consistent and prolonged drug release over time, AI enhances controlled-release medication formulations. Overall, the figure shows how AI-driven modelling and analysis lead to more accurate, effective, and patient-centred treatment approaches.

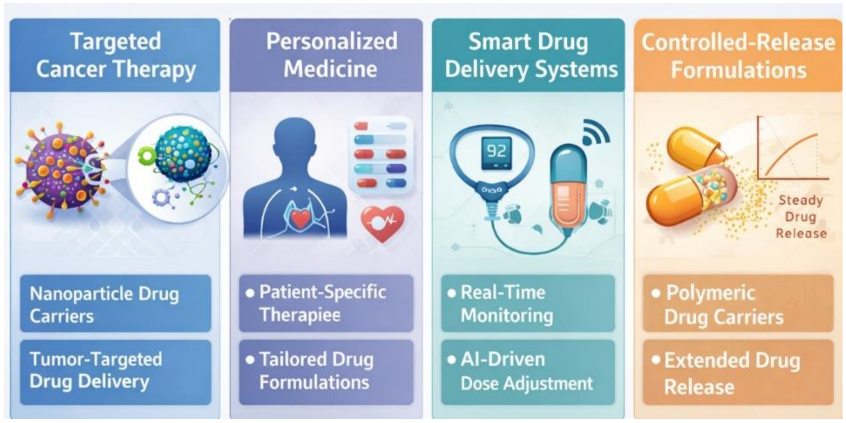

Figure 3. Applications of AI optimised drug delivery

Targeted cancer therapy

One of the most exciting developments in contemporary oncology is AI-driven drug delivery systems. These devices minimise exposure to healthy cells by delivering anticancer medications straight to malignant areas. To create highly tailored nanoparticles for drug administration, AI algorithms can examine a variety of aspects of the tumour microenvironment, including pH levels, receptor expression, vascular density, and metabolic processes. AI aids in the development of delivery systems that enhance drug accumulation at the tumor site by forecasting how these particles will interact with cancer cells. The negative effects of chemotherapy, such as immune suppression, organ damage, and hair loss, are greatly reduced by this focused strategy. As a result, patients enjoy a better quality of life in addition to receiving more effective treatment. AI-assisted nanomedicine is increasingly being explored for the treatment of diseases such as Cancer through advanced targeted drug delivery platforms (Samathoti et al., 2025; Kapoor et al., 2024).

Personalised medicine

The goal of personalised medicine is to customise medical care based on a patient's genetic composition, disease profile, lifestyle, and anticipated response to medication. By evaluating vast amounts of patient data, including genomic sequences, medical records, imaging results, and laboratory findings, artificial intelligence plays a critical role. AI systems can identify the best medication type, dose, and delivery method for every patient by using pattern recognition. This customised strategy minimises adverse medication reactions, which might differ greatly between patients, while optimising therapeutic efficacy. AI-supported personalised medicine makes healthcare more accurate and patient-focused by ensuring that the appropriate patient receives the right therapy at the right time (Harrer et al., 2019; Wu et al., 2024).

Smart drug delivery systems

To enable real-time physiological analysis and adaptive drug release, smart drug delivery systems merge AI algorithms with wearable monitoring platforms, implantable devices, and biosensors. These systems continually gather biological information, such as pH fluctuations, glucose levels, or enzyme activity, and use predictive models to precisely adjust medicine dosage over time. The AI-enabled closed-loop insulin delivery system, which integrates machine learning-based control algorithms with continuous glucose monitoring (CGM), is a prime example. These algorithms greatly lower the risk of hypoglycemia and enhance glycemic stability by predicting glycemic trends and automatically modifying basal or bolus insulin supply. The precision and responsiveness of medication release patterns are further improved by sophisticated computational techniques like reinforcement learning and model predictive control (MPC). Smart delivery systems that enable therapeutic interventions that dynamically adjust to patient-specific biochemical cues in real time are being developed for autoimmune diseases and oncology, in addition to diabetes (Panchpuri et al., 2025; Du et al., 2025). Table 2 shows different applications of AI in the Drug Delivery system.

Table 2. AI Applications in drug delivery systems

Application Area	Drug Delivery Technology	Role of AI	Clinical Impact
Targeted Cancer Therapy	Nanoparticle drug carriers	Predicts optimal nanoparticle size and targeting	Reduces toxicity and improves tumour targeting
Personalized Medicine	Patient-specific drug formulations	Analyses genetic and clinical data	Tailored treatment strategies
Smart Drug Delivery	Biosensor-integrated systems	Real-time analysis and dose adjustment	Improved disease management
Controlled Release Systems	Polymer-based delivery platforms	Predicts drug release kinetics	Sustained therapeutic effects
Clinical Decision Support	AI-assisted dosing models	Optimises treatment protocols	Improved patient outcomes

Future perspectives

Hyperintelligent biomedical ecosystems with the ability to make independent therapeutic decisions will influence the next generation of AI-assisted drug delivery. To mimic whole treatment trajectories before drug administration, future systems will use digital twin constellations that are constantly updated with multi-omics, biomechanical, and environmental data. With almost no latency, these high-resolution virtual copies will enable predictive regulation of drug release and predict negative biological effects. With the help of quantum-accelerated AI models, self-evolving labs will be able to design, produce, and optimise nanocarriers on their own while carrying out millions of in-silico tests every hour. Sentinel nanosystems particles with molecular logic circuits capable of autonomous navigation, biomarker decoding, and intracellular decision-making for precise payload deployment will be the next step in AI-integrated nanomedicine. Complementary innovations will consist of:

- Bioresponsive drug matrices that are 4D printed and change dynamically inside the body.
- Continuous molecular-level diagnostics made possible by holographic IoMT networks.
- Completely self-sufficient therapeutic monitoring systems with self-correcting, anticipatory dosage algorithms.

When taken as a whole, these developments will create a future in which drug delivery is mostly autonomous, adaptive, and predictive.

Conclusion

Predictive modelling, formulation optimisation, and individualised therapy are all made possible by artificial intelligence, which is revolutionising the drug delivery industry. Researchers can create more effective drug delivery systems, shorten development times, and enhance therapeutic results with AI-assisted optimisation. AI could completely transform pharmaceutical research and healthcare delivery when combined with nanotechnology and precision medicine. Even if there are still issues with data quality, regulations, and model transparency, these constraints should be resolved by continued study and technology developments. AI-driven medication delivery systems will be essential to the advancement of contemporary medicine and the enhancement of patient care globally if they continue to be developed.

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Author contributions

Shalini Jaiswal has participated in data collection, analysis, and interpretation, as well as in drafting and revising the manuscript.

Competing interests

The author declares that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Ethics approval

This study did not involve human participants or animals. Therefore, formal ethical approval was not required. All fieldwork and sample collection were conducted in accordance with local regulations and institutional guidelines.

AI Tool Usage Declaration

The authors declare that artificial intelligence tools were used only for language editing and improving the clarity of the manuscript. The authors take full responsibility for the content of the manuscript, including the accuracy of the data, analysis, and conclusions.

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